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Three-dimensional structure of phosphorus-containing heterocycles Communication 33. Oxides and selenides of 2-phenoxy-5,5-dimethyl-1,3,2-dioxaphosphorinanes

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Abstract

1. An analysis of the temperature dependence of the Raman, IR, and PMR spectra and dipole moments of the oxide, sulfide and selenide of 2-phenoxy-5,5-dimethyl-1-3,2-dioxaphosphorinane showed that going from this oxide to the sulfide and selenide is accompanied by a shift in the conformational equilibrium from the ananchimerically displaced equilibrium in the oxide to the presence of both chair forms in the sulfide and selenide. The form which axial, gauche orientation of the phenoxyl group predominates. The less populated conformer has chair form with an equatorial, gauche phenoxy group. 2. The UV spectral data indicates that the structure found in the oxide and selenide are such that p-π conjugation of the unshared p electron pair of the exocyclic oxygen atom which the π-electrons of the benzene ring is hindered. © 1985 Plenum Publishing Corporation.

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